TECHNISCHE UNIVERSITÄT DRESDEN

DLR

German Aerospace Center (DLR) Institute of Software Methods for Product Virtualization - Dresden

Quantum Approaches to Partial Differential Equations: A Comparative Study of the Variational Quantum Algorithm and the Imaginary Time Evolution Method

Johanna A. Berger [1,2], Pia Siegl [2,3], Prof. Sabine Roller [1,2]

[1] German Aerospace Center (DLR), Institute of Software Methods for Product Virtualization, Dresden, Germany
[2] Institude of Artificial Intelligence - Chair of Software Methods for Product Virtualization, Faculty of Computer Science, Dresden University of Technology, Dresden, Germany
[3] Institute for Quantum Physics, University of Hamburg, Hamburg, Germany

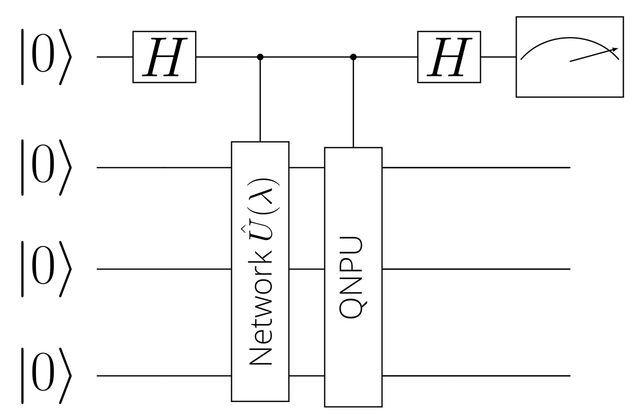
Motivation The problem of solving differential equations is foundational to our understanding of the natural and engineered world. From the turbulence in aerodynamics and biochemical diffusion processes to market dynamics in quantitative finance, many complex phenomena can be described by partial differential equations (PDEs). Yet, classical solvers face steep computational costs, especially for nonlinear or high-dimensional problems. Quantum computing, with its intrinsic parallelism and vast state space, offers a promising new route toward more efficient PDE solutions. This study investigates two promising quantum methods for solving partial differential equations (PDEs), Variational Time Stepping (VTS) and Imaginary Time Evolution (ITE). This work is focused on their foundational principles, algorithmic performance, and suitability for near-term quantum architectures.

Theory

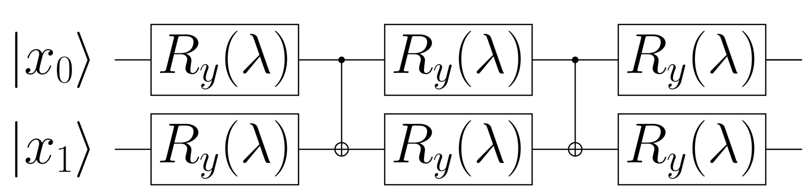
Methode 1: Variational Time Stepping (VTS) [1]

1. **Encode finite-difference operators on a QNPU** [1]
   Map spatial derivatives to quantum nonlinear processing unit (QNPU)
2. **Apply the Variational Time-Stepping (VTS) method**
   Learn time stepping by minimizing residuals of the PDE variationally.
3. **Hybrid quantum–classical training**
   Classical optimizer updates quantum parameters iteratively.

Time Evolution: $argmin_\lambda C(\lambda)$ with $C \ldots$ cost function



Variational circuit



Variational brick $\hat{U}(\lambda_1)$

Method 2: Quantum Imaginary Time Evolution (QITE) [2], [3]

The Simulated Quantum Imaginary Time evolution uses the Hamiltonian to encode the differential operators, leading to the ground state being the normalized solution of the PDE. The approach applies Trotter steps to approximate the imaginary time evolution operator in small intervals.

QITE Trotter Step: $e^{-i\hat{A}\Delta\tau}|\psi(\tau)\rangle \approx \frac{e^{-\hat{h}_I\Delta\tau}|\psi(\tau)\rangle}{\sqrt{\langle\psi(\tau)|e^{-2\hat{h}_I\Delta\tau}|\psi(\tau)\rangle}}$

1. **Hamilton encoding of the differential operator**
2. **Imaginary time propagation**
   For each time step $\Delta\tau$, apply the non-unitary update $e^{-\Delta\tau\hat{H}}$, approximated via Trotterization.
3. **Reconstruct norm**
   After every step approximate norm and correct resulting error after k steps

Benchmarking Metrics

$$\text{MSE} = \sqrt{\frac{\sum_j (u_j^{\text{quantum}} - u_j^{\text{exact}})^2}{\sum_j (u_j^{\text{exact}})^2}} \qquad \text{Error}_{\text{Max}} = \max_j |u_j^{\text{quantum}} - u_j^{\text{exact}}|$$

Problem Setup

One Dimensional Diffusion Equation

$\partial u/\partial t = \partial u/\partial x + v$
model for fundamental transport phenomena (e.g. fluid dynamics, environmental sciences, biochemistry, …) and an analytical solution available for benchmarking

Initial Condition: Gaussian profile

Encoding: $|\Psi\rangle = \frac{1}{\sqrt{\sum_{k=0}^{N-1}|u_k|^2}} \sum_{k=0}^{N-1} u_k |k\rangle$

Implementation Details

Simulation Parameters

Parameters	Value Range
Qubits (n)	6
VTS Layers	7
ITE Trotter Steps	[40, 100, 200]
Time Step (Δt)	0.01

Quantum simulations were performed using Pennylane (v0.36) with JAX-based optimization, employing the default.qubit backend. Adam and LBFGS optimizers ensured stable hybrid quantum-classical convergence for VTS.

Results - Simulated Wavefunctions

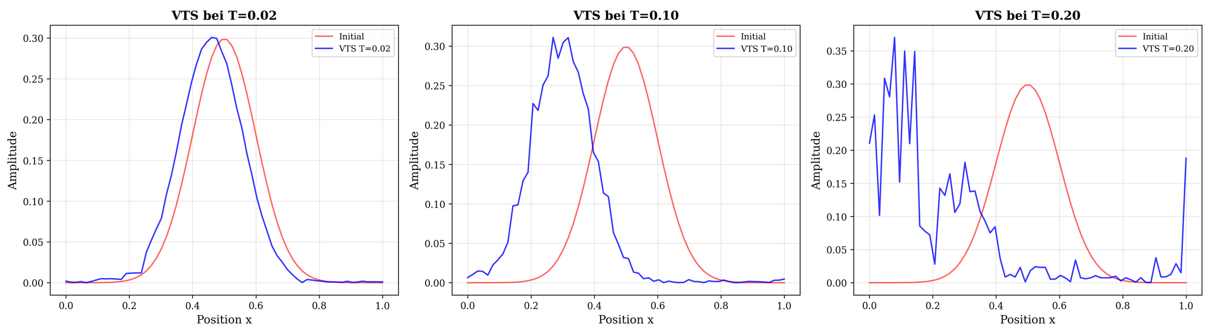


Figure 1: VTS with different time steps [0.02, 0.10, 0.20]

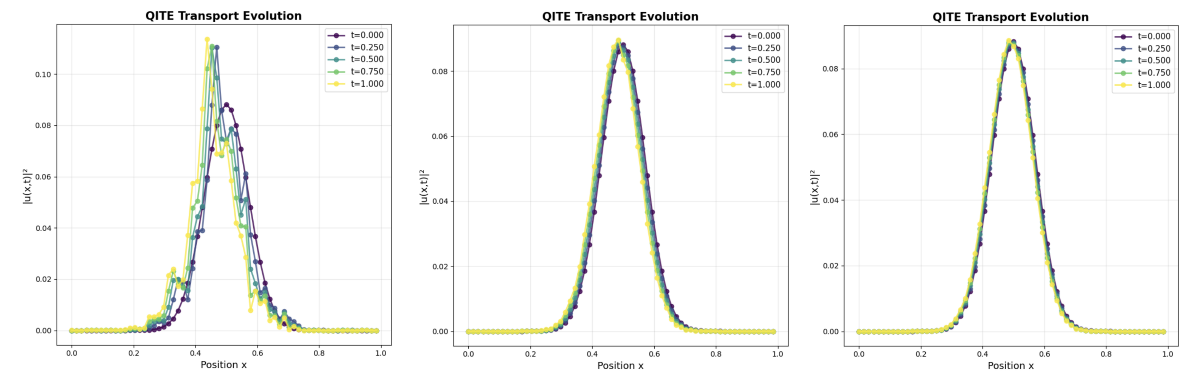


Figure 2: QITE with diffrent Trotter steps [40, 100, 200] for $t = 1$

Method Comparison

When to Use VTS	When to Use ITE
Nonlinear PDEs (Burgers, Navier-Stokes)	Linear PDEs with Hamiltonian structure
Flexible boundary conditions via penalty terms	Higher accuracy requirements
Shallower circuits through tensor networks (better for NISQ)	Theoretical guarantees for convergence
Disadvantages:	
Sensitive to variational brick, parameters, and optimizer choice	Deeper circuits (Trotterization overhead)

Ongoing Work

1. Extend the comparison framework
2. Testing robustness of simulation in the presence of noise
3. Scale to 8-12 qubits (N=256-4096 grid points) on HPC with GPU
4. Extend to 2D and other PDEs (e.g. heat equation)

References

[1] M. Lubasch, J. Joo, P. Moinier, M. Kiffner, and D. Jaksch, "Variational quantum algorithms for nonlinear problems", en, *Physical Review A*, vol. 101, no. 1, Jan. 2020, Publisher: American Physical Society (APS), ISSN: 2469-9926, 2469-9934. DOI: `10.1103/physreva.101.010301`. Accessed: Jul. 13, 2025.

[2] M. Motta et al., "Determining eigenstates and thermal states on a quantum computer using quantum imaginary time evolution", *Nature Physics*, vol. 16, no. 2, pp. 205–210, Nov. 2019, ISSN: 1745-2481. DOI: `10.1038/s41567-019-0704-4`.

[3] S. Kumar and C. M. Wilmott, "Generalising quantum imaginary time evolution to solve linear partial differential equations", May 2024, arXiv: 2405.01313. DOI: `10.1038/s41598-024-70423-5`.